Benzo[b]thiophene-4-ol

Other names: Benzo[b]thiophene-4-ol
4-Hydroxybenzothiophene
1-Benzothiophene-4-ol
Inchi: InChI=1S/C8H6OS/c9-7-2-1-3-8-6(7)4-5-10-8/h1-5,9H
InchiKey: BMRZGYNNZTVECK-UHFFFAOYSA-N
Formula: C8H6OS
SMILES: Oc1cccc2sccc12
Mol. weight [g/mol]: 150.20

Physical Properties

Property code	Value	Unit	Source
hf	-32.48	kJ/mol	Cheméo Relay (1.0)
ie	7.61	eV	Cheméo Relay (1.0)
log10ws	-2.42		Cheméo Relay (1.0)
logp	2.607		Crippen Method
mcvol	106.880	ml/mol	McGowan Method
tb	547.88	K	Cheméo Relay (1.0)
tf	408.49	K	Cheméo Relay (1.0)

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3610024&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

hf: Enthalpy of formation at standard conditions

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point